

Supporting Information

Characterization and quantification of isoprene-derived epoxydiols in ambient aerosol in the southeastern United States

Man Nin Chan¹, Jason, D. Surratt², Magda Claeys³, Eric S. Edgerton⁴, Roger L. Tanner⁵, Stephanie L. Shaw⁶, Mei Zheng⁷, Eladio M. Knipping⁸, Nathan C. Eddingsaas², Paul O. Wennberg^{1,9}, and John H. Seinfeld^{*,1,2}

¹Division of Engineering and Applied Science, California Institute of Technology, Pasadena, California, USA.

²Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California, USA.

³Department of Pharmaceutical Sciences, University of Antwerp, Antwerp, Belgium.

⁴Atmospheric Research and Analysis, Inc., Cary, North Carolina, USA.

⁵Environmental Technologies, Tennessee Valley Authority, Muscle Shoals, Alabama, USA.

⁶Electric Power Research Institute, Palo Alto, California, USA.

⁷School of Earth and Atmospheric Sciences, Georgia Institute of Technology, Atlanta, Georgia, USA.

⁸Electric Power Research Institute, Washington, DC, USA.

⁹Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, California, USA

*To whom correspondence should be addressed. email: seinfeld@caltech.edu

Number of Page: 3

Number of Table: 5

Table S1. Averaged gas-phase concentrations in downtown Atlanta, GA (JST) and a rural location in Yorkville, GA (YRK) during the 2008 AMIGAS campaign ^a

JST										
Sampling date	August 9, 2008		August 24, 2008 to August 26, 2008 (Rain period) ^b		September 3, 2008		September 5, 2008		September 6, 2008	
	Day	Night	Day	Night	Day	Night	Day	Night	Day	Night
O ₃	76	16	22	12	60	7.8	56	0.2	45	10
CO	191	392	164	131	187	549	161	668	165	216
SO ₂	2.4	3.2	1.0	1.0	1.4	2.3	0.6	3.0	16	0.3
NO	0.7	2.0	4.5	3.6	2.6	35	1.1	43	0.5	0.7
NO ₂	3.6	28	9.4	7.7	9.2	30	5.0	36	4.0	12
YRK										
Sampling date	August 12, 2008		August 13, 2008		September 6, 2008					
	Day	Night	Day	Night	Day	Night				
O ₃	51	34	60.2	21	39	13				
CO	188	235	186	185	146	155				
SO ₂	3.5	1.3	7.2	0.5	1.0	0.1				
NO	0.6	0.0	0.2	0.2	0.2	0.1				
NO ₂	3.5	4.4	0.8	1.9	0.6	1.6				

^a Averaged gas-phase concentrations are reported in ppb.

^b For the rain period, averaged gas-phase concentrations are reported from August 24, 2008 to August 26, 2008.

Table S2. The major fragment ions observed in the EI mass spectrum of trimethylsilylated IEPOX formed from the photooxidation of isoprene in the presence of acidified sulfate seed aerosol under low-NO_x conditions at retention time (RT) = 23.23 min (Figure 1b)

Measured mass	Calculated mass	Formula	mDa
262.1418	262.1421	C ₁₁ H ₂₆ O ₃ Si ₂	-0.3
218.1147	218.1158	C ₉ H ₂₂ O ₂ Si ₂	-1.1
147.0663	147.0661	C ₅ H ₁₅ OSi ₂	0.2
131.0896	131.0892	C ₆ H ₁₅ OSi	0.4
130.0808	130.0814	C ₆ H ₁₄ OSi	-0.6
117.0722	117.0736	C ₅ H ₁₃ OSi	-1.4
116.0656	116.0657	C ₅ H ₁₂ OSi	-0.1
101.0427	101.0423	C ₄ H ₉ OSi	0.4

Table S3. The major fragment ions observed in the EI mass spectrum of trimethylsilylated IEPOX formed from the photooxidation of isoprene in the presence of acidified sulfate seed aerosol under low-NO_x conditions at RT = 23.73 min (Figure 1c)

Measured mass	Calculated mass	Formula	mDa
262.1414	262.1421	C ₁₁ H ₂₆ O ₃ Si ₂	-0.7
248.1145	218.1158	C ₉ H ₂₂ O ₂ Si ₂	-1.3
147.0655	147.0661	C ₅ H ₁₅ OSi ₂	-0.6
131.0873	131.0892	C ₆ H ₁₅ OSi	-1.9
130.0811	130.0814	C ₆ H ₁₄ OSi	-0.3
117.0733	117.0736	C ₅ H ₁₃ OSi	-0.3
116.0659	116.0657	C ₅ H ₁₂ OSi	0.2
101.0426	101.0423	C ₄ H ₉ OSi	0.3

Table S4. The major fragment ions observed in the EI mass spectrum of trimethylsilylated IEPOX in fine atmospheric aerosol collected during the daytime on August 9, 2008 at JST at RT = 23.35 min (Figure 1e)

Measured mass	Calculated mass	Formula	mDa
262.1408	262.1421	C ₁₁ H ₂₆ O ₃ Si ₂	-1.3
218.1133	218.1158	C ₉ H ₂₂ O ₂ Si ₂	-2.5
147.0676	147.0661	C ₅ H ₁₅ OSi ₂	1.5
131.0923	131.0892	C ₆ H ₁₅ OSi	3.1
130.0810	130.0814	C ₆ H ₁₄ OSi	-0.4
117.0725	117.0736	C ₅ H ₁₃ OSi	-1.1
116.0657	116.0657	C ₅ H ₁₂ OSi	0
101.0424	101.0423	C ₄ H ₉ OSi	0.1

Table S5. The major fragment ions observed in the EI mass spectrum of trimethylsilylated IEPOX in fine atmospheric aerosol collected during the daytime on August 9, 2008 at JST at RT = 23.86 min (Figure 1f)

Measured mass	Calculated mass	Formula	mDa
262.1436	262.1421	C ₁₁ H ₂₆ O ₃ Si ₂	1.5
218.1127	218.1158	C ₉ H ₂₂ O ₂ Si ₂	-3.1
147.0663	147.0661	C ₅ H ₁₅ OSi ₂	0.2
131.0921	131.0892	C ₆ H ₁₅ OSi	2.9
130.0830	130.0814	C ₆ H ₁₄ OSi	1.6
117.0722	117.0736	C ₅ H ₁₃ OSi	-1.4
116.0652	116.0657	C ₅ H ₁₂ OSi	-0.5
101.0422	101.0423	C ₄ H ₉ OSi	-0.1